Sustainable Computing for Fluid Dynamics via Physics-Informed Surrogates

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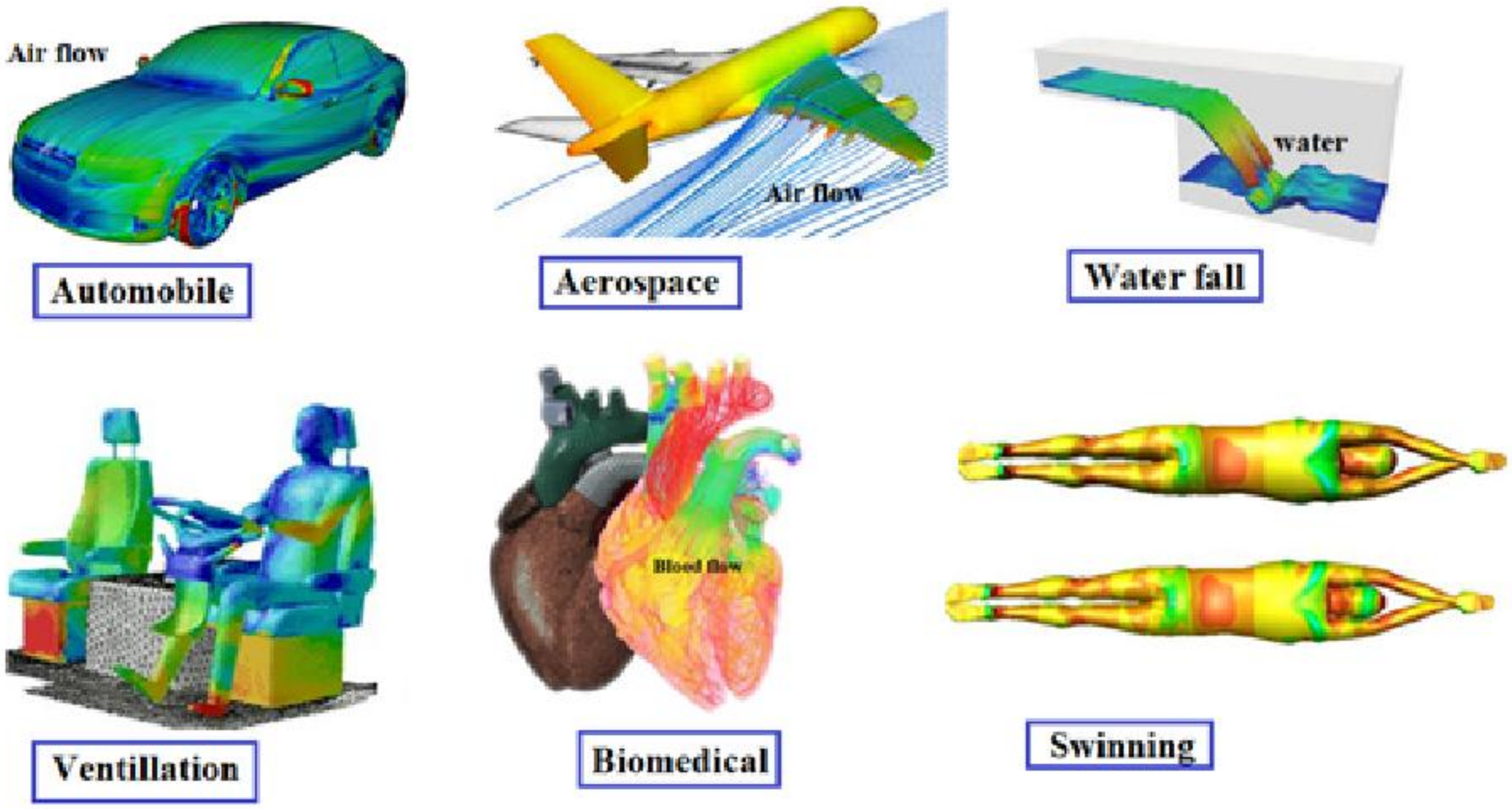
w/Luigi Ciceri, Corrado Mio, Jianyi Lin

Green ICT & ICT for Green Workshop, 29 October 2025
ECSS 2025 - European Informatics Leaders Summit, Rennes

Computational Fluid Dynamics (CFD)

- CFD is the field of numerical simulation of flow-related problems
- It finds application in a number of diverse domains



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Review

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http://dx.doi.org/10.1098/rsta.2013.0317

One contribution of 13 to a Theme Issue 'Aerodynamics, computers and the environment'.

Subject Areas:
environmental engineering

Enabling the environmentally clean air transportation of the future: a vision of computational fluid dynamics in 2030

Jeffrey P. Slotnick[1], Abdollah Khodadoust[1], Juan J. Alonso[2], David L. Darmofal[3], William D. Gropp[4], Elizabeth A. Lurie[5], Dimitri J. Mavriplis[6] and Venkat Venkatakrishnan[7]

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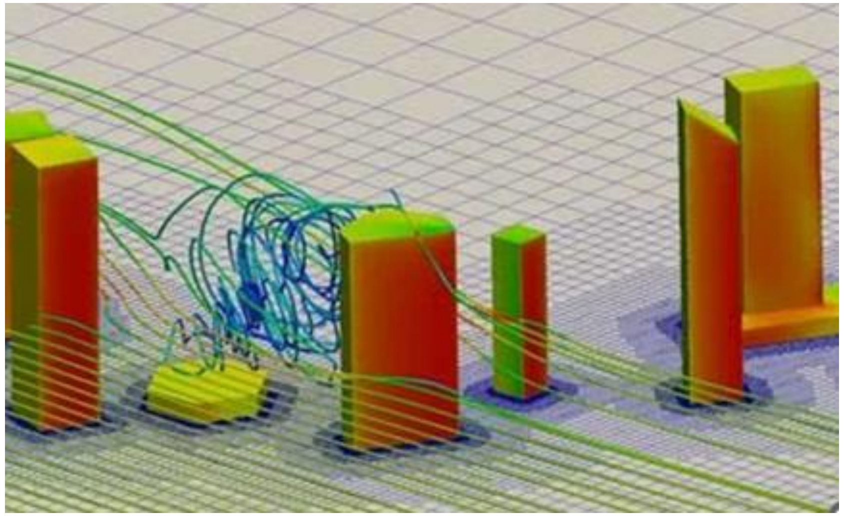
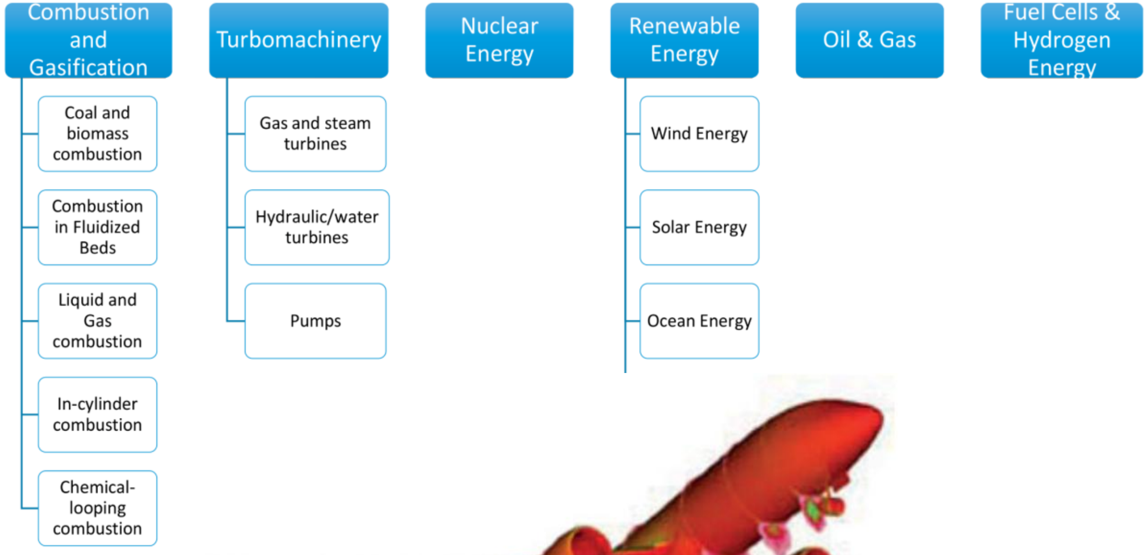
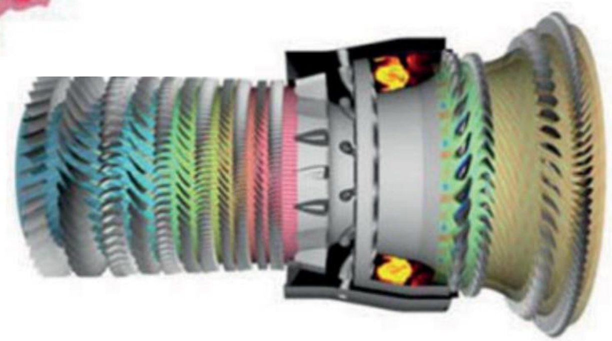




Large Eddy Simulation

Turbo engine Digital Twins



Key role in the design of efficient transportation, as well as urban landscapes design

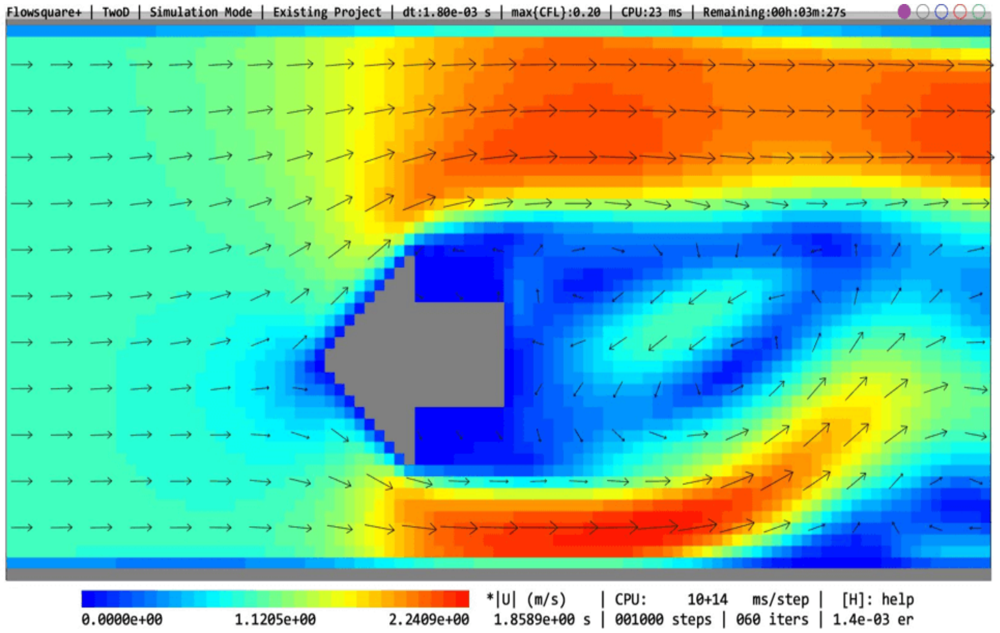
The task

Numerically **predicting behavior of fluids**

- Motion, forces, transport of heat/mass/momentum

By solving the governing physical equations, e.g. **Navier-Stokes'** under given

- <u>Geometry</u>/domain
- Physical <u>params:</u> **ρ** (density), **μ** (viscosity)…
- Boundary conditions <u>(BCs)</u>
- Initial conditions (<u>ICs</u> for transient problems)
  - Inlet fields (velocity/mass-flow, temperature)
  - Outlet fields (pressure/zero-gradient)
  - Walls (no-slip/slip, heat flux/temperature…)
- <u>Forcing</u> (volumetric sources):
  - gravity/buoyancy, porous drag



<u>Numerics</u> (implicit but important): discretization (FVM/FEM), mesh/resolution, time stepping, solver tolerances

Navier-Stokes Partial Differential Equations

- Often the target quantities are
  - Velocity vector field v(x,y,z), Pressure field p(x,y,z),
- And the equations are the Navier-Stokes PDEs, e.g. for v and p

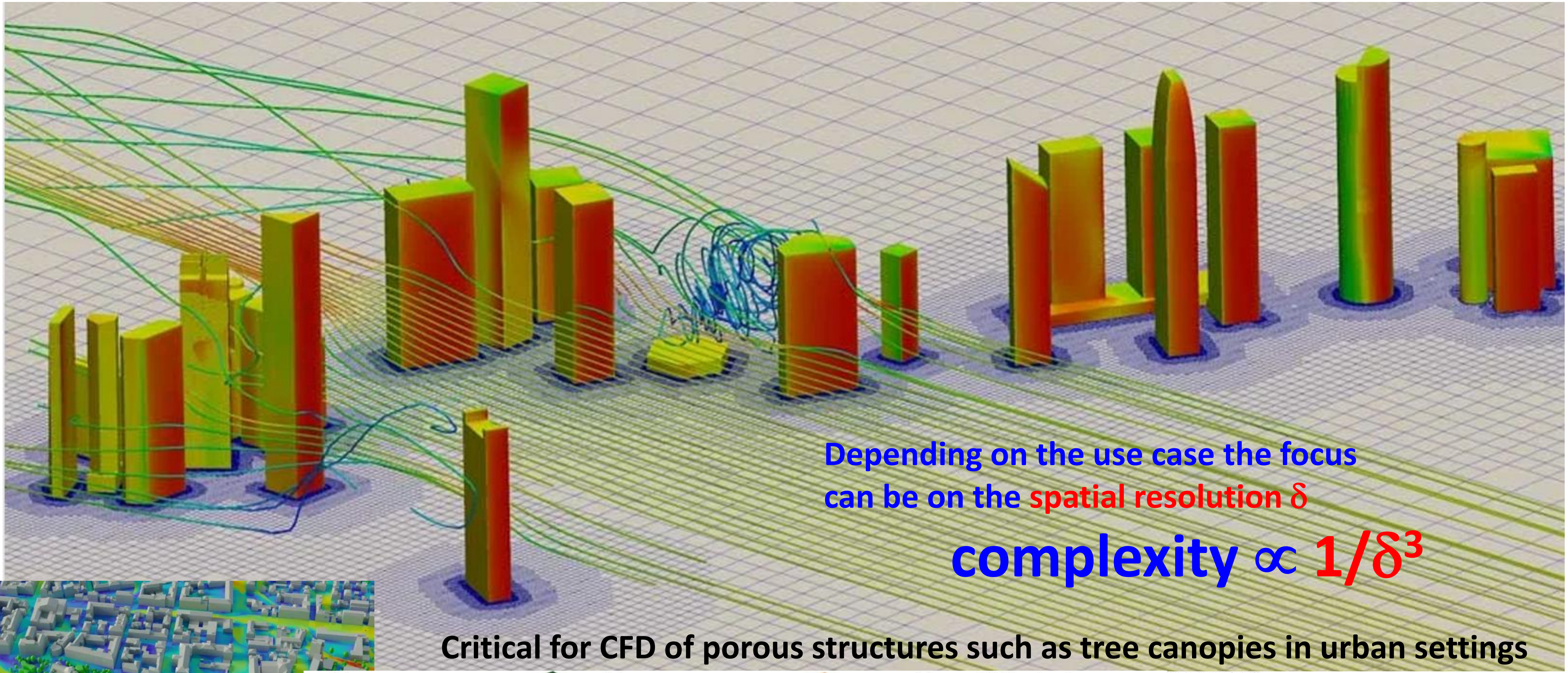
$$\overbrace{\underbrace{\rho}_{\text{Density of the Fluid}}}^{\text{MASS}} \cdot \overbrace{\left(\underbrace{\frac{\partial \vec{\mathbf{v}}}{\partial t}}_{\text{Change in Velocity over Time}} + \underbrace{(\vec{\mathbf{v}} \cdot \nabla)\vec{\mathbf{v}}}_{\text{Speed and Direction of Fluid}}\right)}^{\text{ACCELERATION}} = \overbrace{\underbrace{\rho\vec{\mathbf{g}}}_{\text{External Forces such as Gravity}} - \underbrace{\nabla p}_{\text{Pressure Gradient}} + \underbrace{\mu \cdot \nabla^2 \vec{\mathbf{v}}}_{\text{Internal Stress Forces (viscous effects)}}}^{\text{FORCE}}$$

Space discretization

FDE
FVM
FEM

Steady incompressible, no forcing case

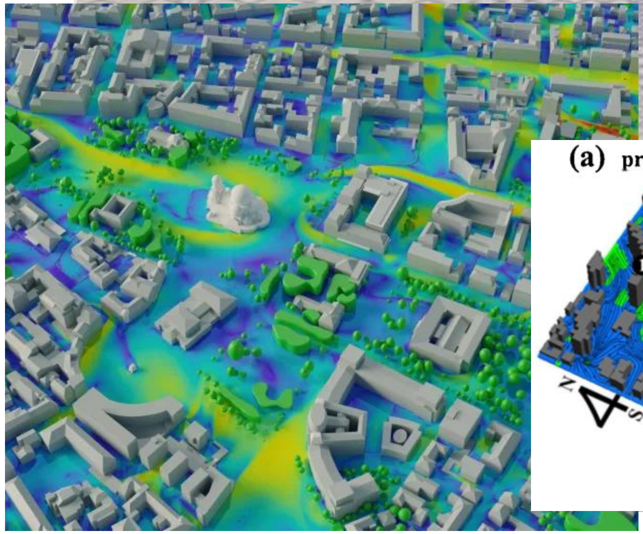
$$\rho(\mathbf{v} \cdot \nabla)\mathbf{v} = -\nabla p + \mu \nabla^2 \mathbf{v}$$

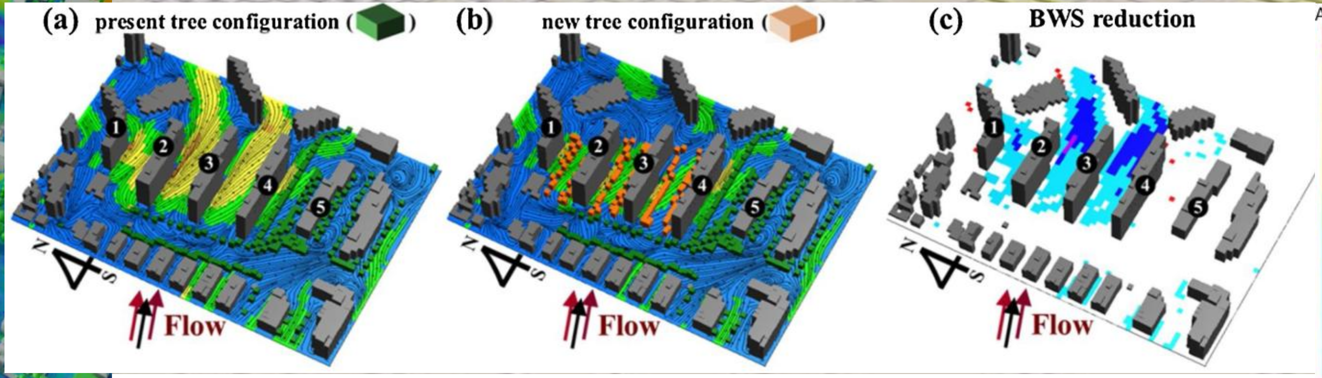


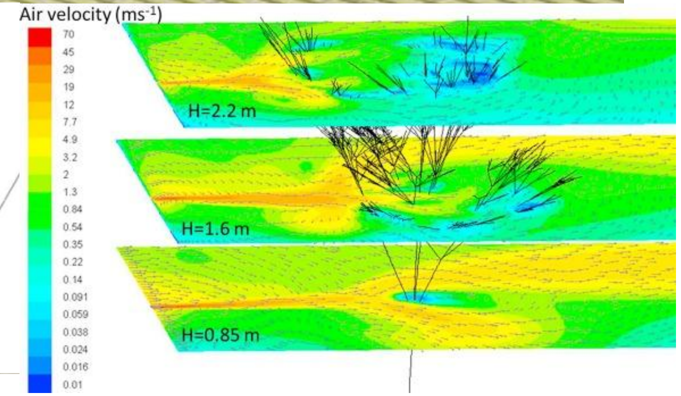
Depending on the use case the focus can be on the spatial resolution δ

complexity $\propto 1/\delta^3$

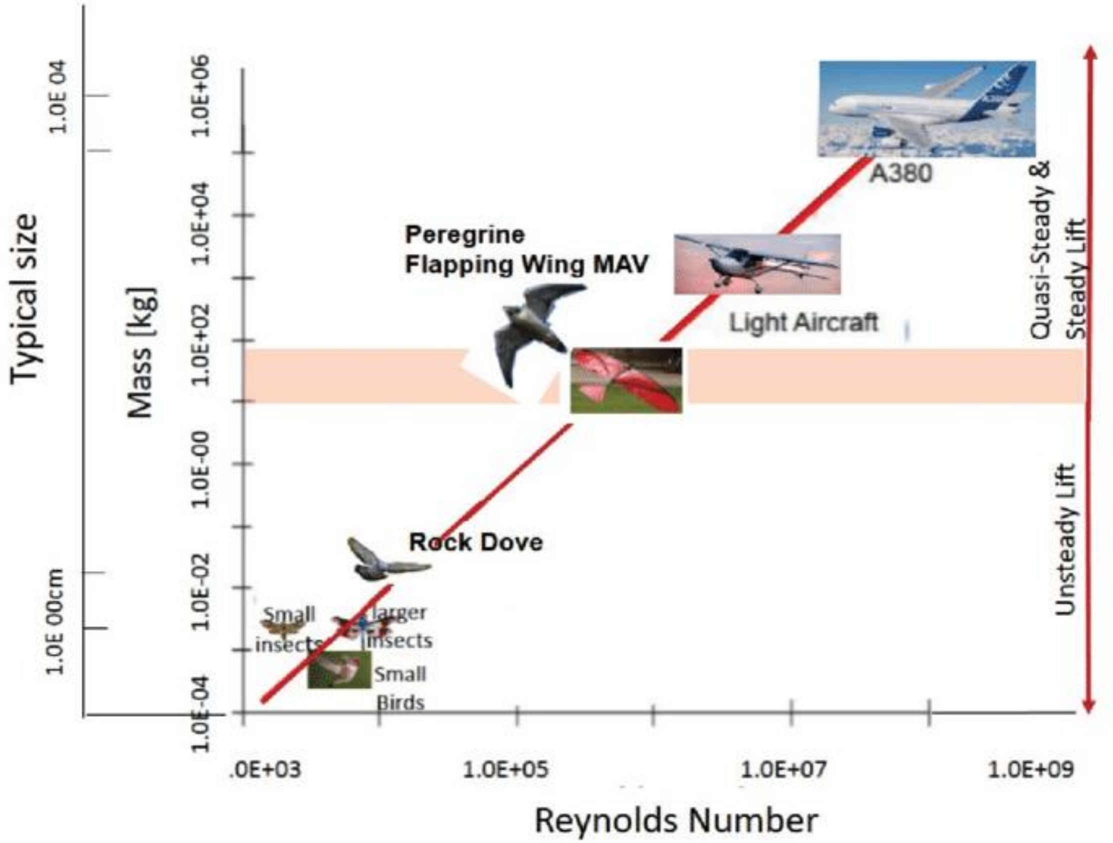
Critical for CFD of porous structures such as tree canopies in urban settings

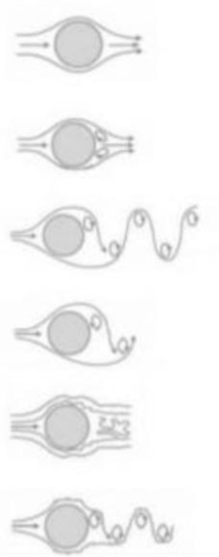






Laminar vs. Turbolent flows





Flow pattern	Reynolds number	Description
	$Re < 5$	No separation, laminar steady flow
	$5 < Re < 45$	Pair of vortices, laminar steady flow
	$45 < Re < 150$	Laminar vortex street, unsteady flow
	$150 < Re < 3 \cdot 10^5$	Transitional unsteady flow
	$3 \cdot 10^5 < Re < 3 \cdot 10^6$	Turbulent unsteady flow
	$Re > 3 \cdot 10^6$	Turbulent vortex street, unsteady flow

https://www.idealsimulations.com/resources/reynolds-number/

These PDEs can become hard to solve in particular parameter ranges, especially with high → more turbolent systems, roughly **Reynolds number**

$$Re = \frac{Inertial\ Force}{Viscous\ Force} = \frac{\rho V L}{\mu}$$

comput. complexity $\propto Re^{3\text{-}4}$

Re from 1 to 10^9

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Volume 16, Issue 5

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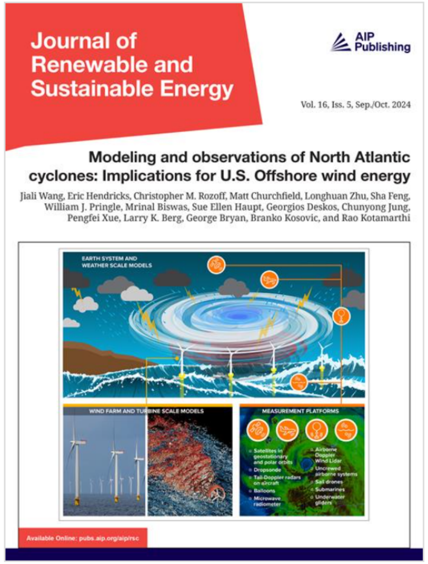

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RESEARCH ARTICLE | OCTOBER 23 2024 https://doi.org/10.1063/5.0217320

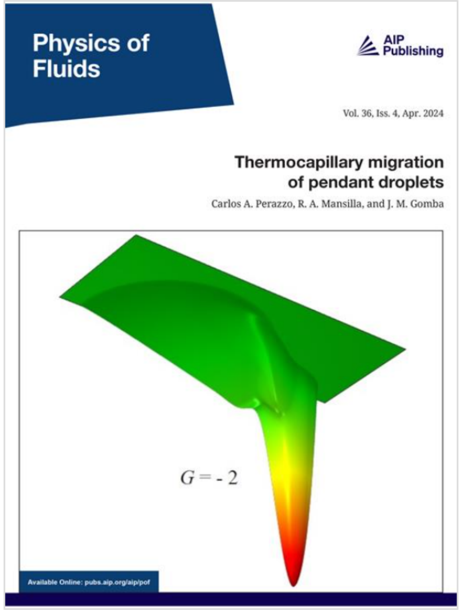
Computational fluid dynamics: Its carbon footprint and role in carbon reduction

Special Collection: Flow, Turbulence, and Wind Energy

Xiang Yang; Wen Zhang; Mahdi Abkar; William Anderson

Volume 36, Issue 4

April 2024



RESEARCH ARTICLE | APRIL 02 2024 https://doi.org/10.1063/5.0199350

Estimating the carbon footprint of computational fluid dynamics

J. A. K. Horwitz

Check for updates

+ Author & Article Information

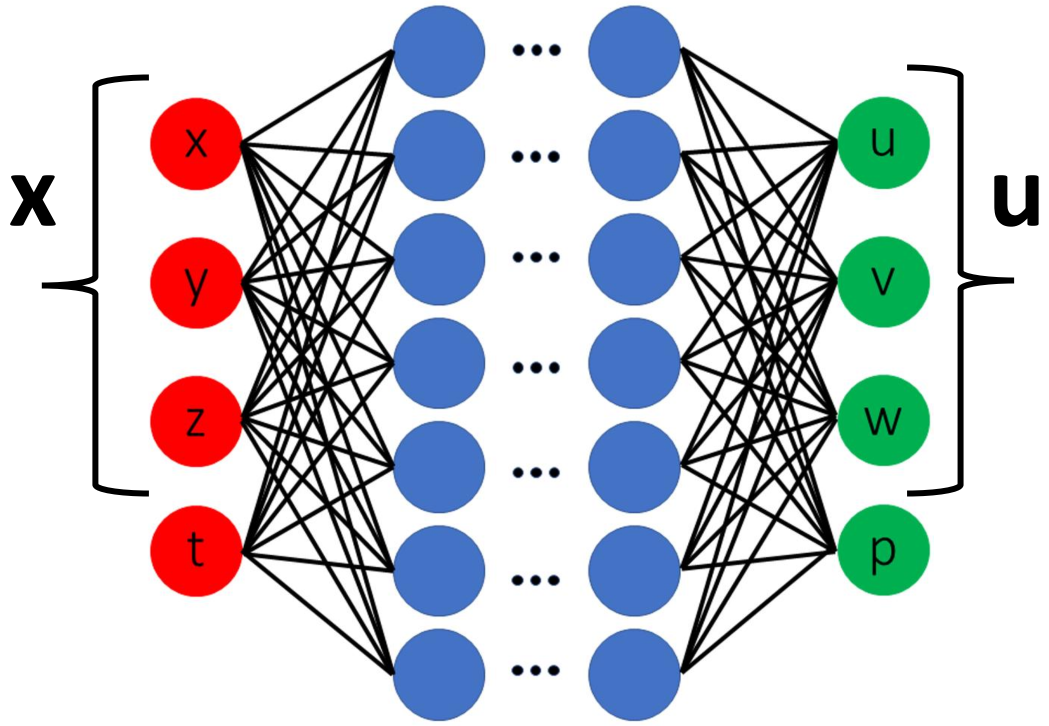
Physics of Fluids 36, 045109 (2024)

Order-of-magnitude estimated examples:

footprint **10^4 kg of CO_2** for single run

- dependent on year, hw efficiency, PUE grid

Deep Learning approach: ANN as CFD surrogates



A typical Green Computing approach

Teacher-Student pattern

Trainig ANN with data from CFD runs

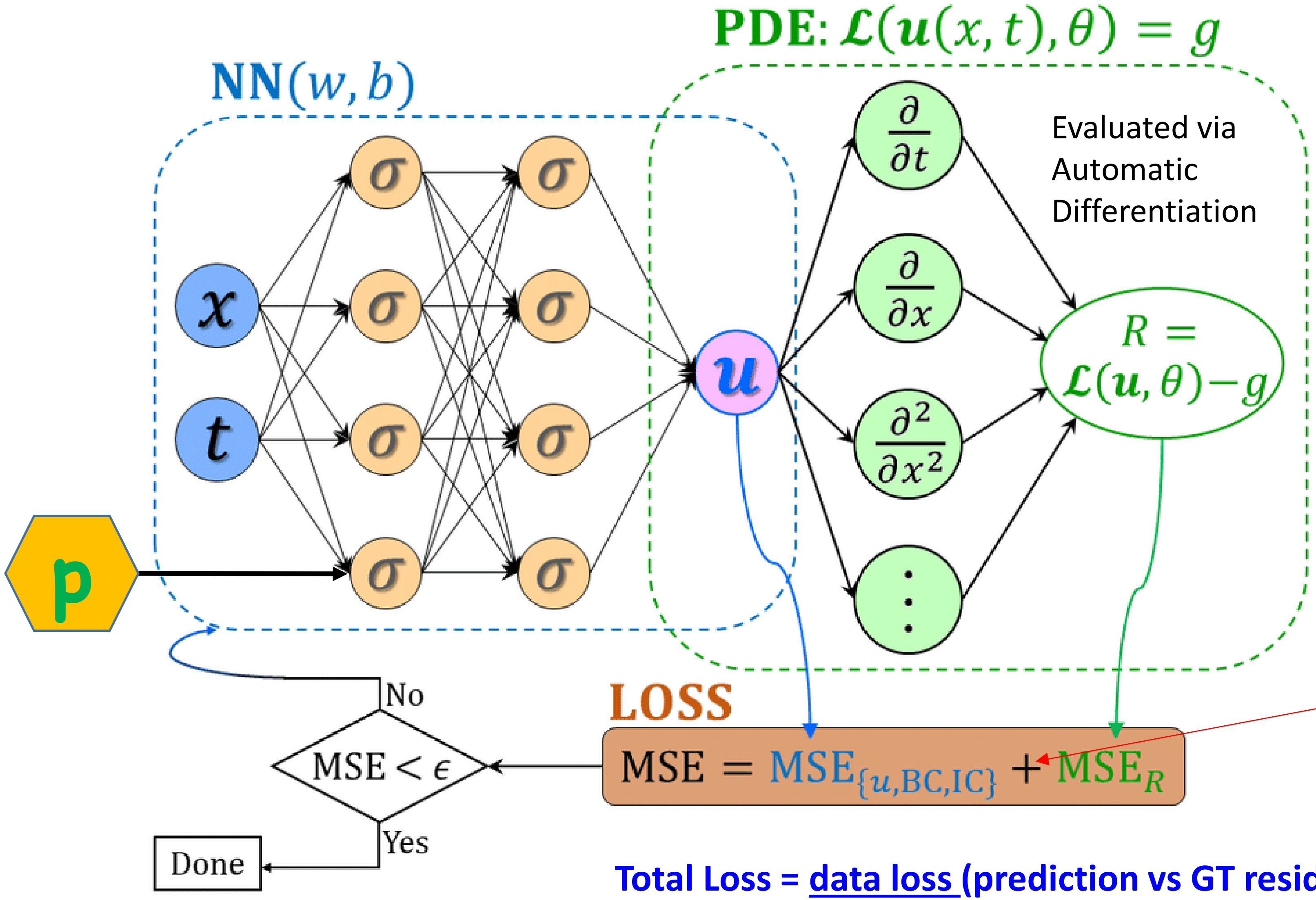
UP SIDE: can learn complex patterns

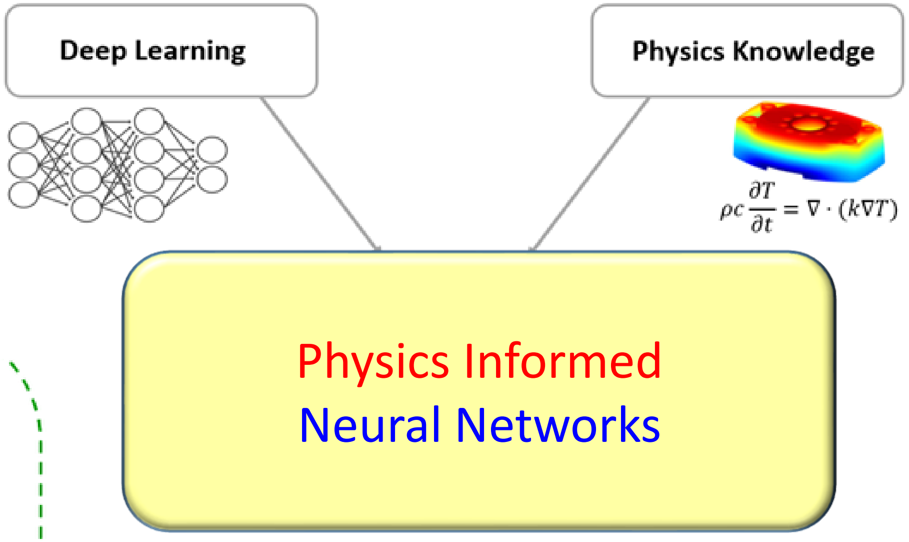
DOWN SIDE:

- Without physics in the loss/architecture
  - ANNs waste data learning the laws,
  - lack conservation awareness
  - and collapse outside their training bubble
- Data hungry!

Physics Informed Neural Networks (PINNs)

Loss = Data loss + Physics loss



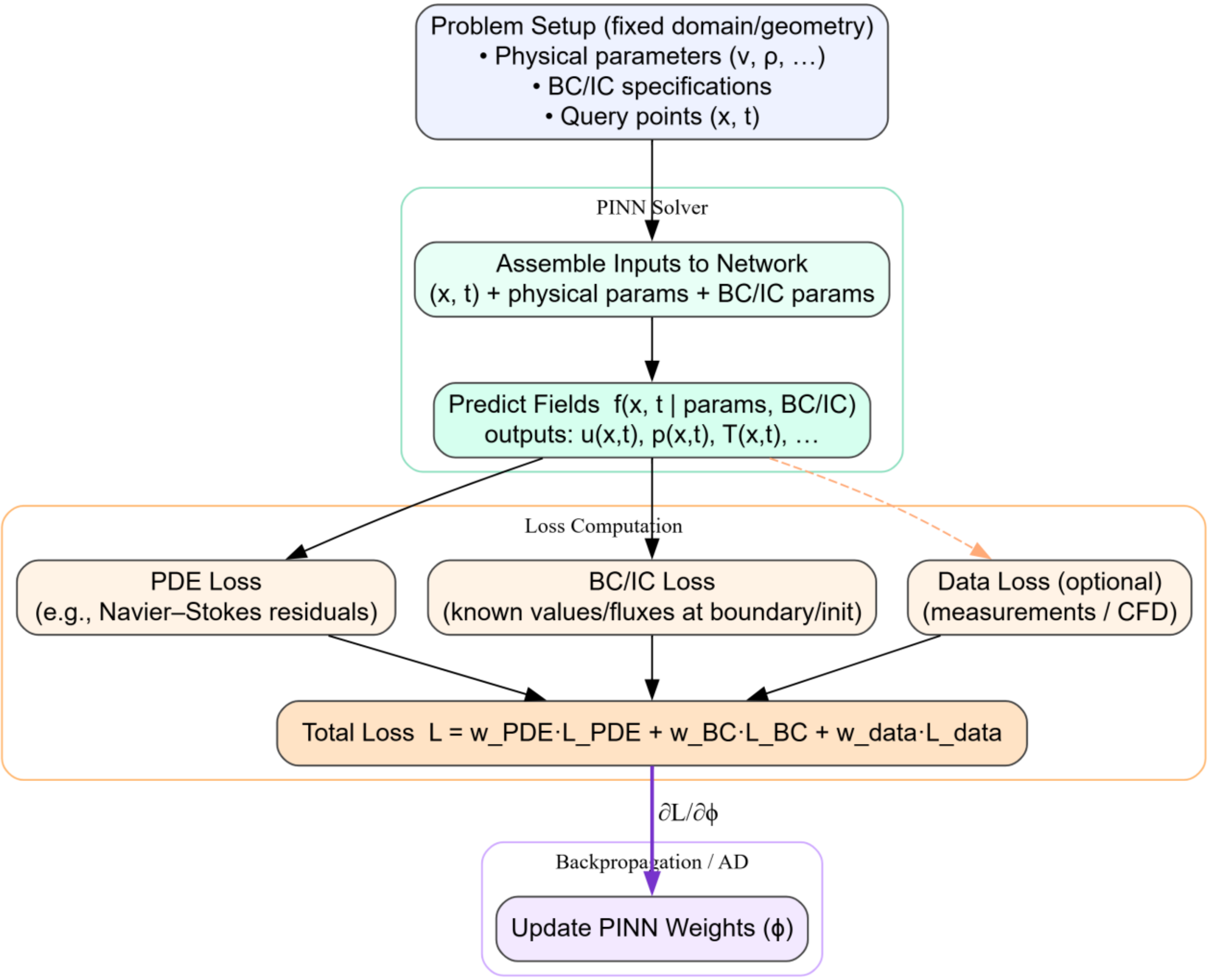


$$L_e = \frac{1}{N_e} \sum_{i=1}^{3} \sum_{n=1}^{N_e} |\epsilon_i^n|^2,$$ Residual of the RANS equations (Unsupervised loss)

$$L_b = \frac{1}{N_b} \sum_{n=1}^{N_b} |\mathbf{U}_b^n - \tilde{\mathbf{U}}_b^n|^2,$$ Loos for the BCs (Supervised loss)

Total Loss = data loss (prediction vs GT residuals) + Physics loss (PDE residuals/BC)

PINNs learn $u_\theta(x , t | p)$



Predict u() conditional to/generalizing over

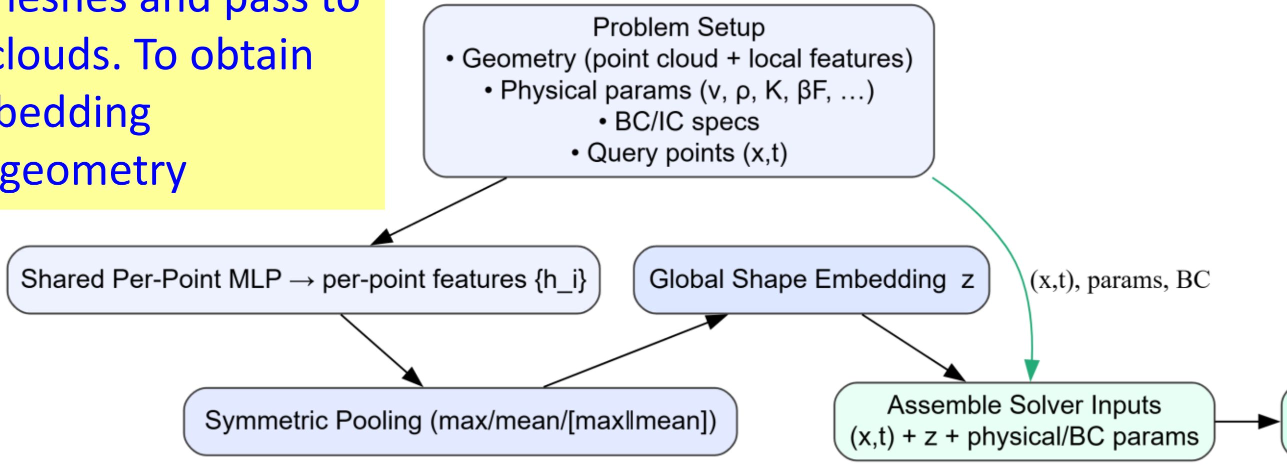
- Initial Conditions/Boundary Conditions
- Physical parameters θ: ν, ρ, K, β_F
- Adding **p** = {BC/IC/θ} as inputs to ANN and sampling on hypercube
  - interpolation **OK**,
  - extrapolation **fragile**

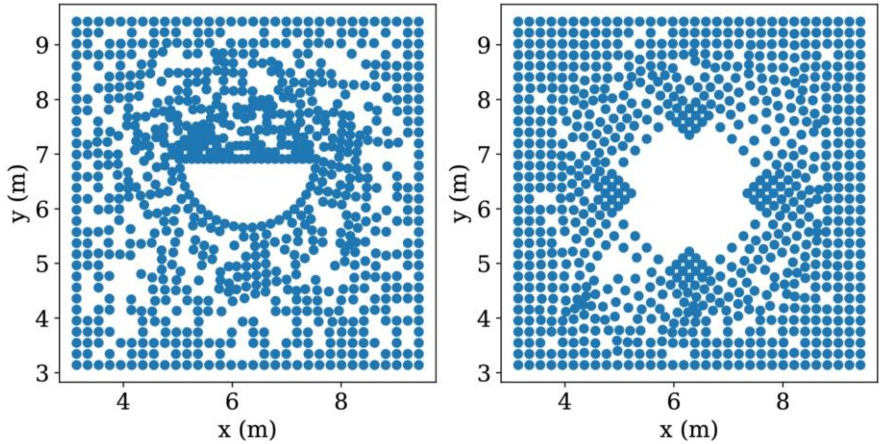
Domain Geometry is Hardcoded

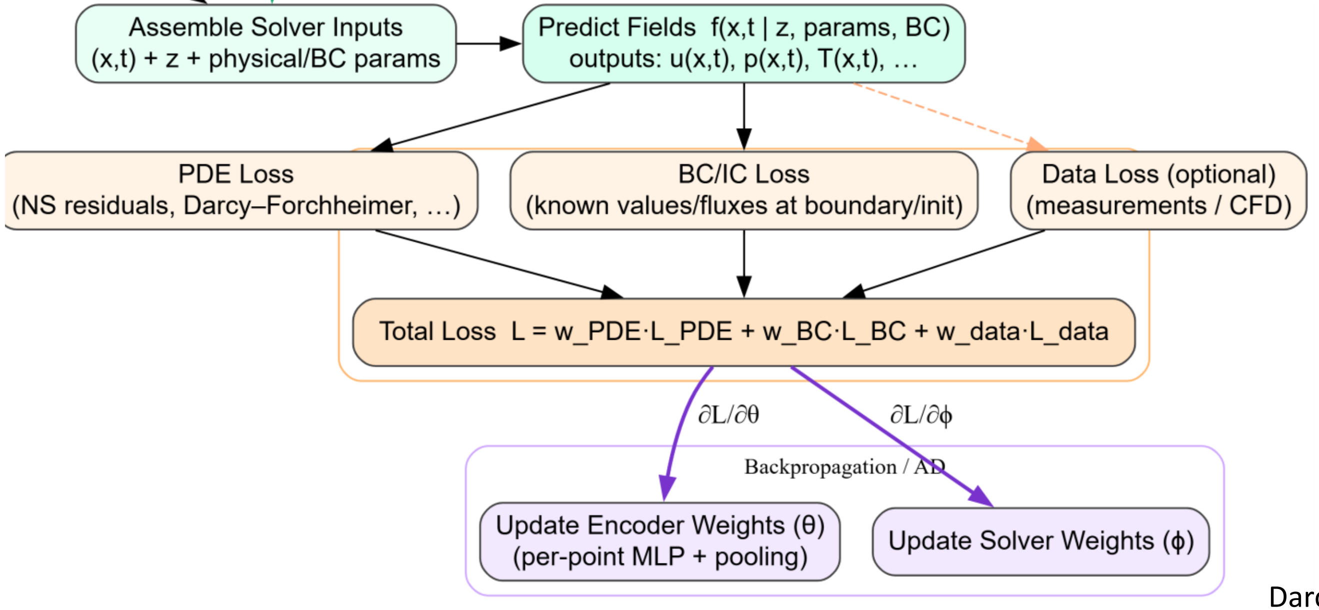
- Possible geometrical awareness via inclusion of geomety parametrization in **p**: **limited**
- **Must retrain for every new geometry!**

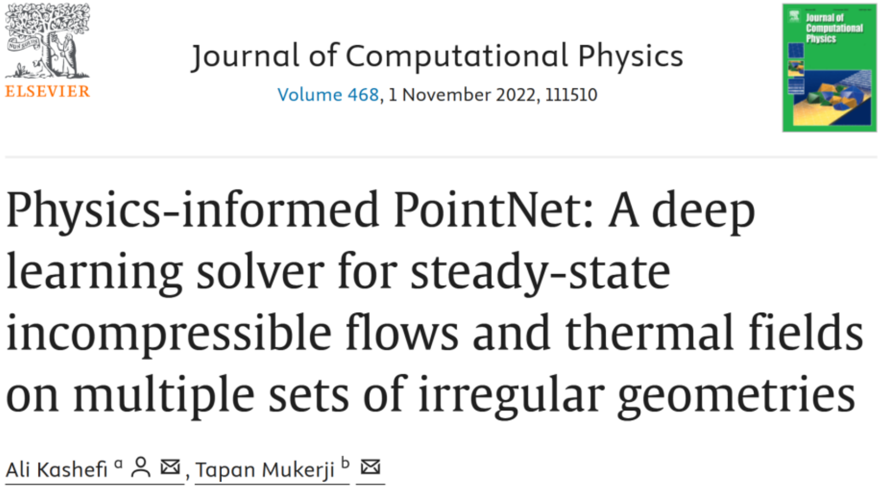
PI-PointNets add geometry awareness via point-clouds

Drop meshes and pass to point clouds. To obtain an embedding of the geometry









ELSEVIER
Journal of Computational Physics
Volume 468, 1 November 2022, 111510

Physics-informed PointNet: A deep learning solver for steady-state incompressible flows and thermal fields on multiple sets of irregular geometries

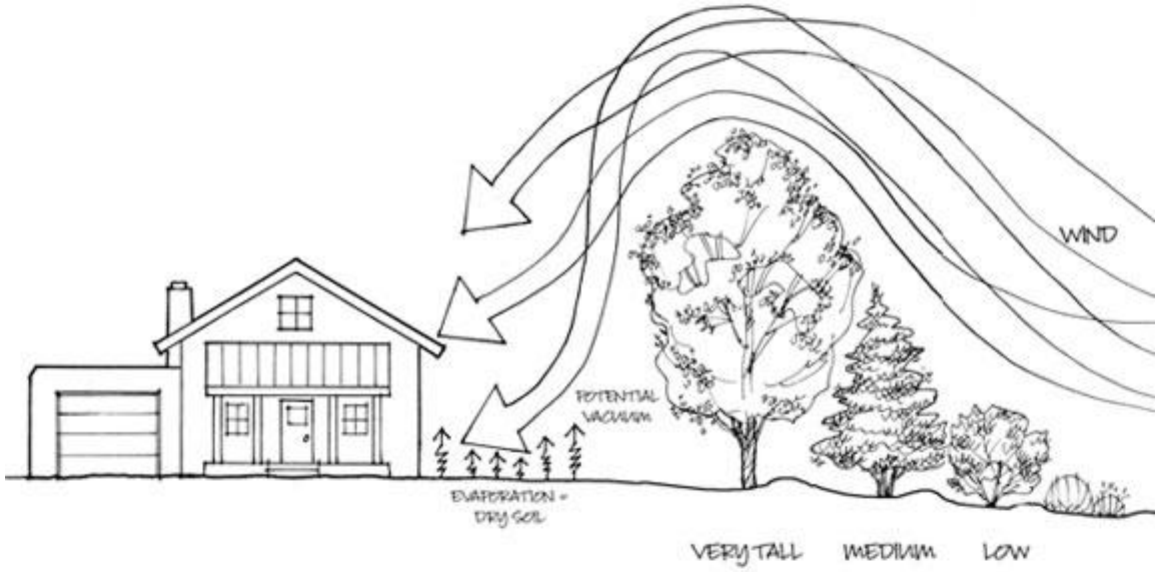
Ali Kashefi [a], Tapan Mukerji [b]

We applied **PIPointNets** to **hybrid free flow and porous medium** materials

$$\underbrace{\rho(\mathbf{v}\cdot\nabla)\mathbf{v} = -\nabla p + \mu\nabla^2\mathbf{v}}_{\text{Navier-Stokes for incompressible fluid}} - \overbrace{\left(\mu D + \frac{1}{2}\rho F|\mathbf{v}|\right)\mathbf{v}}^{\text{Darcy-Forcheimer}}$$

Porous regions

- Flows that occur both **through and around** porous bodies at different scales are central to applications such as
- submerged breakwaters,
- rock-filled gabions,
- industrial filters,
- catalytic beds,
- heat exchangers
- coral reefs
- plant canopies
- **windbreaks** such as
    - vegetation barriers, fences, and perforated facades of buildings, used in various environmental and <u>wind mitigation applications</u>.



PI-GANOs map geometry via operators

Computer Methods in Applied Mechanics and Engineering
Volume 434, 1 February 2025, 117540

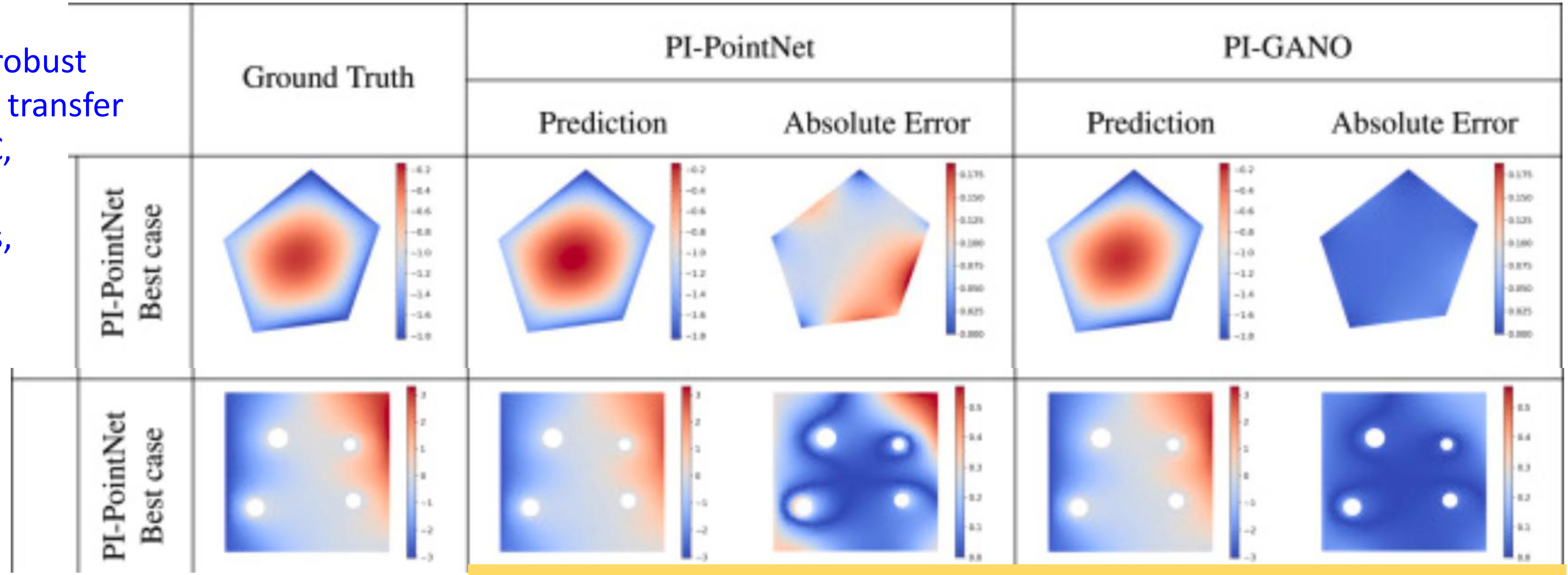
Physics-Informed Geometry-Aware Neural Operator

Weiheng Zhong, Hadi Meidani

From PIPN to PIGANO you move

- from a “geometry-conditioned solution function”
- to “a geometry-aware neural operator,”
  - learns a map between function spaces: input fields (coefficients/forcing/BC/geometry) to the solution field of a PDE, using layers that act on **functions** rather than finite-dimensional vectors

This enables robust zero/few-shot transfer across new BC, parameters, discretizations, geometry and forcing



We applied PIGANOs to hybrid freeflow and porous medium materials

Our architecture: from PI-PointNet++ to PI-GANO++

If accuracy degrades at sharp interfaces/ geometry has fine, multi-scale details one one can move **from PIPN to PIPN++**

- PIPN++ upgrades the encoder to a hierarchical, locality-aware version, adding multi-scale neighborhood features and local conditioning

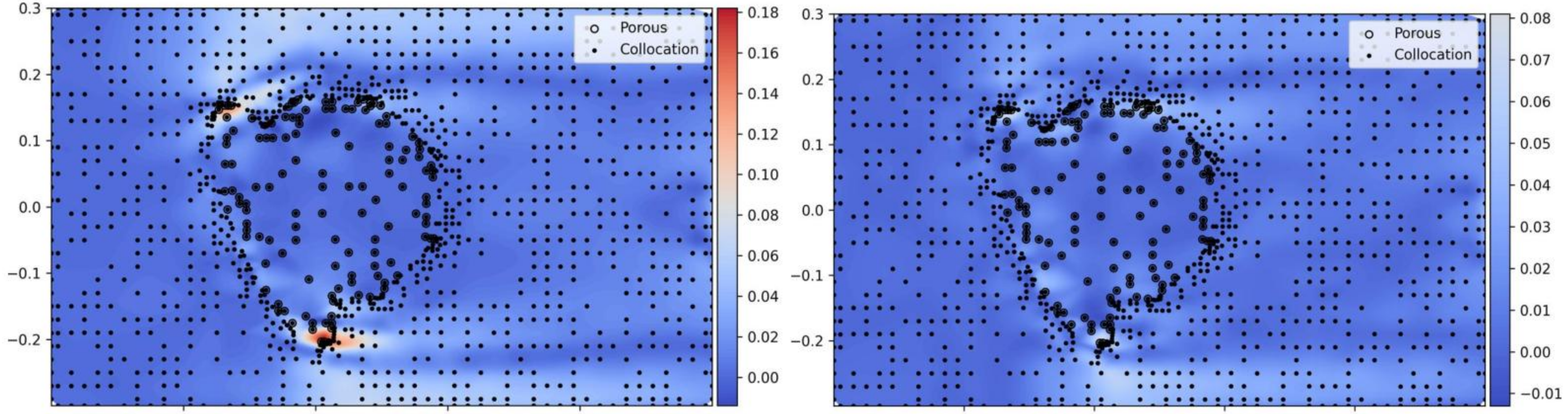
We performed the same operation with **PIGANO** developing a **PIGANO++** architecture, which in analogy to PIPN++ brings

- hierarchical, locality-aware geometry into the neural-operator setting

Yields better boundary/interface fidelity and generalization to fine geometric details—without giving up neural-operator flexibility across BCs, parameters, and meshes.

Our work:
- developed PIGANO++
- applied PIPN++ and PIGANO++ to hybrid freeflow and porous medium materials

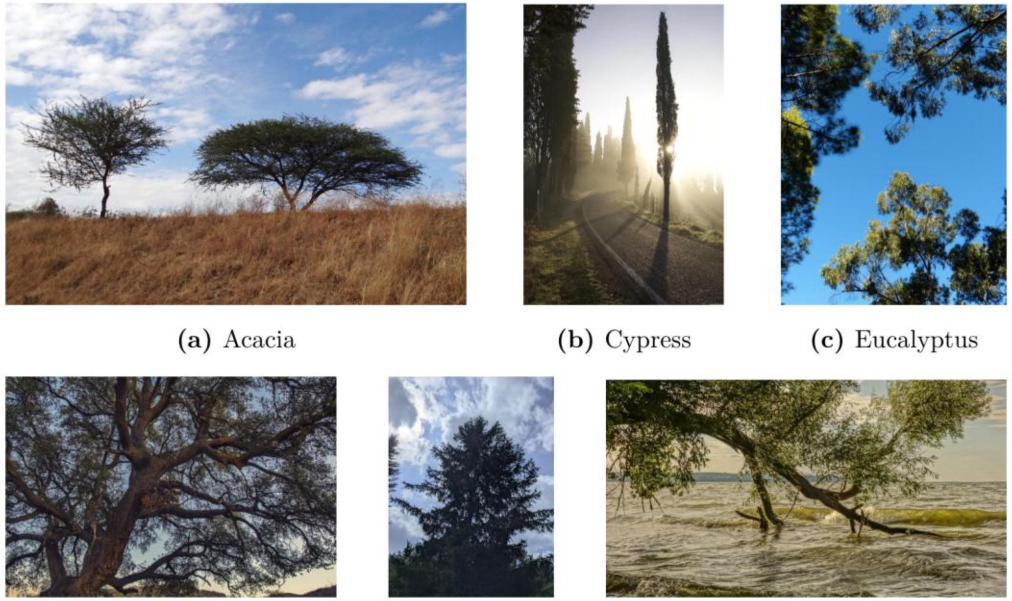
Example with 2D porous shape: PIPN++



(a) PIPN (b) PIPN++ MRG

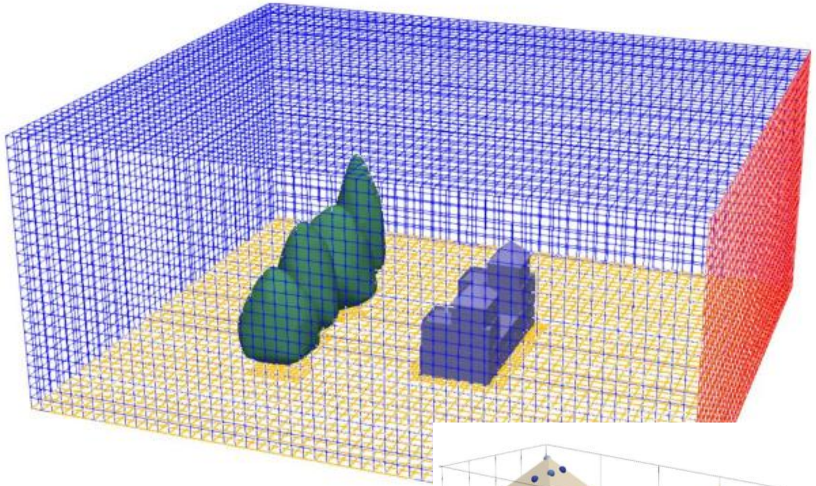
Error landscape

MAE in windbreak case studies



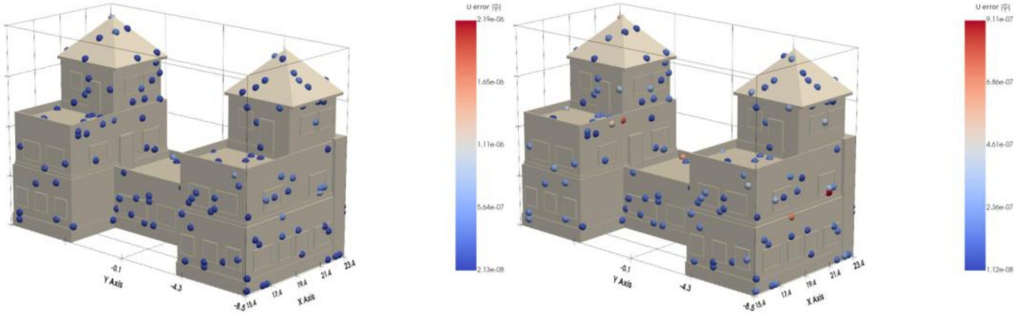
(a) Acacia (b) Cypress (c) Eucalyptus

(d) Oak (e) Pine (f) Willow



inlet, ground and outlet

(b) P



(a) PI-GANO (b) PI-GANO++

	U_x		U_y		U_z		p	
Model	P.G.	P.G.++	P.G.	P.G.++	P.G.	P.G.++	P.G.	P.G.++
Total	$1.15 \cdot 10^{-7}$	$\mathbf{9.83 \cdot 10^{-8}}$	$4.15 \cdot 10^{-8}$	$\mathbf{3.66 \cdot 10^{-8}}$	$3.23 \cdot 10^{-8}$	$\mathbf{3.02 \cdot 10^{-8}}$	$2.37 \cdot 10^{-12}$	$\mathbf{2.36 \cdot 10^{-12}}$
Solid	$8.86 \cdot 10^{-8}$	$\mathbf{8.70 \cdot 10^{-8}}$	$3.89 \cdot 10^{-8}$	$\mathbf{3.87 \cdot 10^{-8}}$	$2.56 \cdot 10^{-8}$	$\mathbf{2.50 \cdot 10^{-8}}$	$3.52 \cdot 10^{-12}$	$\mathbf{3.27 \cdot 10^{-12}}$
Porous	$\mathbf{1.39 \cdot 10^{-7}}$	$1.60 \cdot 10^{-8}$	$\mathbf{4.57 \cdot 10^{-8}}$	$5.02 \cdot 10^{-8}$	$\mathbf{5.06 \cdot 10^{-8}}$	$5.60 \cdot 10^{-8}$	$\mathbf{7.05 \cdot 10^{-12}}$	$7.32 \cdot 10^{-12}$
Fluid	$1.14 \cdot 10^{-7}$	$\mathbf{9.51 \cdot 10^{-8}}$	$4.13 \cdot 10^{-8}$	$\mathbf{3.59 \cdot 10^{-8}}$	$3.13 \cdot 10^{-8}$	$\mathbf{2.88 \cdot 10^{-8}}$	$2.12 \cdot 10^{-12}$	$\mathbf{2.09 \cdot 10^{-12}}$
Max	$\mathbf{2.09 \cdot 10^{-6}}$	$2.45 \cdot 10^{-6}$	$\mathbf{9.21 \cdot 10^{-7}}$	$9.62 \cdot 10^{-7}$	$\mathbf{9.39 \cdot 10^{-7}}$	$1.06 \cdot 10^{-6}$	$8.69 \cdot 10^{-11}$	$\mathbf{8.51 \cdot 10^{-11}}$

Average Times $\quad \mathrm{CO_{2e}} = \mathrm{PUE} \cdot P_{\mathrm{IT}} \cdot T \cdot \mathrm{CI}$

Method	Mesh / Collocation	Training Time (x factor CFD)	Inference Time (per case)
OpenFOAM (Laminar)	86 k cells	-	26 min 20.4 min
PIPointNets	2500 pts	**110** min (**4.23**)	12 ms
PIGANO	3000 pts	**301** min (**14.75**)	14 ms
PIGANO++	3000 pts	**309** min (**15.15**)	17 ms

HW: HPC cluster, 32 CPU cores + NVIDIA A100

(2D) ABC for PIPN, (3D) windbreaks for PI-GANO & PI-GANO++

MEDES 2025 - The 17th International Conference on Management of Digital Ecosystems (Ho Chi Min city, VT)

Geometry-Aware Physics-Informed PointNets for Modeling Flows Across Porous Stuctures

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Questions?